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Title: Nuclear Modeling of (n, x, gamma) Reactions & Determination of Partial Cross Sections

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Los Alamos
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ABSTRACT

"Nuclear modeling of (n,x gamma) reactions and determination of partial cross sections"

This talk would describe nuclear reaction modeling work in collaboration with experimental measurements at Los Alamos' GEANIE array. The GEANIE array is able to measure discrete gamma-rays in the deexcitation of residual nuclei produced following neutron-induced reactions, using time-of-flight with a white neutron spectrum. We have studied reactions on a range of target nuclides including actinides (e.g. 239Pu, 235,8U) as well as dosimetry materials (e.g. Y89, 193Ir). Since GEANIE is unable to measure all deexcitation gamma-rays, nuclear modeling and theory is needed to augment the measurements. This allows the gamma-ray data to be understood in terms of direct, preequilibrium, Hauser-Feshbach, fission, and capture mechanisms, and allows reaction channel cross sections to be inferred. The work also involves a study of the excitation of isomers, and reactions on nuclei away from stability, in nuclear reactions.

Nuclear modeling of (n,x γ) reactions & Determination of partial cross sections

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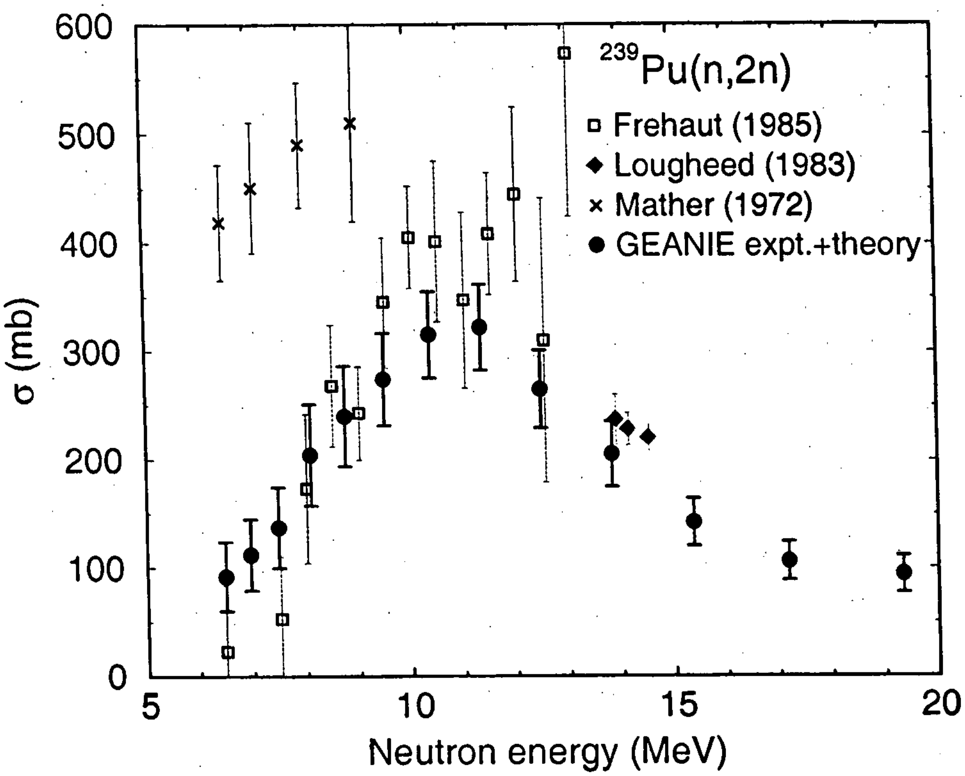
Principal collaborators: Marshall Blann, Ron Nelson, Paul Garrett, Patrick Talou, Pavel Oblozinsky, Phil Young

Overview:

- *LANSCE (n,xγ) experiments*
- *Nuclear model calculations (GNASH, HMS)*
- *Recent work on ^{239}Pu, ^{193}Ir, ^{89}Y,Zr,^{235m}U, Mo, Pt*
- *Angular momentum conservation; HMS preequilibrium*

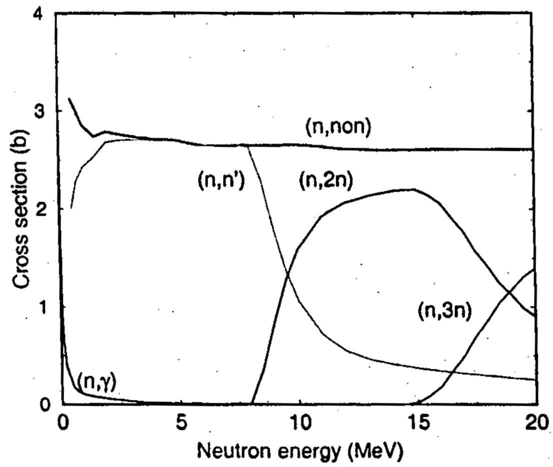
$^{239}Pu(n,2n)^{238}Pu$



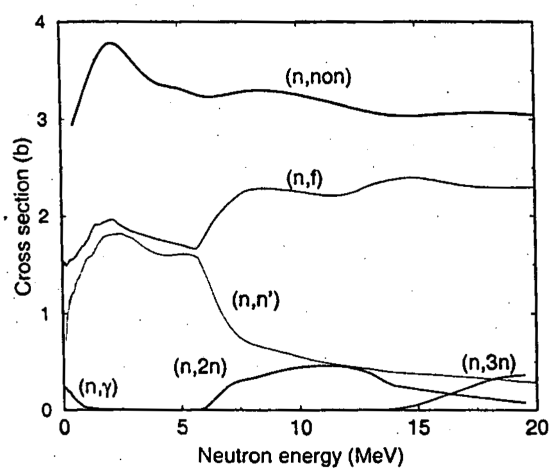
- Previous ^{239}Pu$(n, 2n)$ data discrepant
- New approach uses both experiment and theory
- GEANIE experiment measures characteristic partial γ-rays in ^{238}Pu
- Theory predicts fraction of measured to total $(n, 2n)$
- We also study n+^{235}U reactions as a surrogate for Pu

Why a-priori theory calculations fail for 239Pu(n,2n):
The reaction x/s is not known precisely; & the fission x/s is large

n+^{193}Ir cross sections



n+^{239}Pu ENDF/B-VI cross sections



- For a non-fissionable heavy nucleus, the (n,2n) x/s is a large fraction of the total reaction x/s
- For plutonium, fission is a large cross section, and (n,2n) is small
- Small uncertainties in the nonelastic (reaction) cross section lead to large uncertainties in (n,2n)

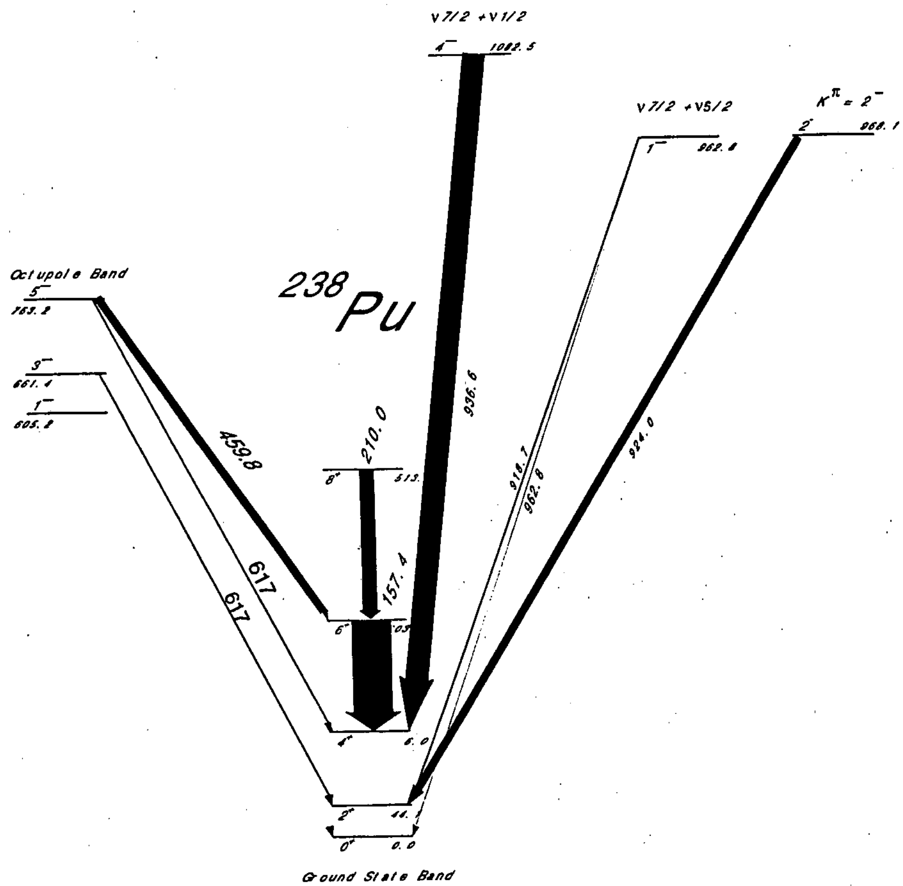
Nuclear theory

Los Alamos: MBC and Phil Young, T-16. The final results are based on the Los Alamos calculations.

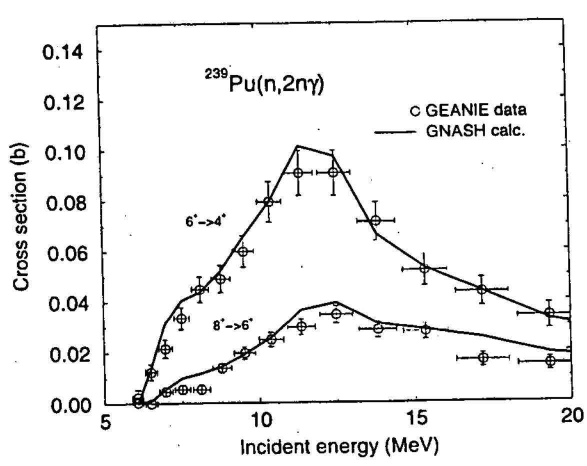
- **Extensive previous experience in modeling and evaluating reactions on actinides**
- **Tested our codes against previous LANSCE/WNR measurements of $(n, xn\gamma)$; extensive work on modeling isomer production**

Livermore: Frank Dietrich, Hong Chen, Erich Ormand.

- **Provided peer-review to LANL theory**
- **Determined that the original LLNL modeling codes unreliable. After LLNL adopted a new code, we have been able to obtain identical results between LANL and LLNL codes using the same input parameters**



GEANIE
LLNL/LANL



Theory: competition between fission and neutron decay

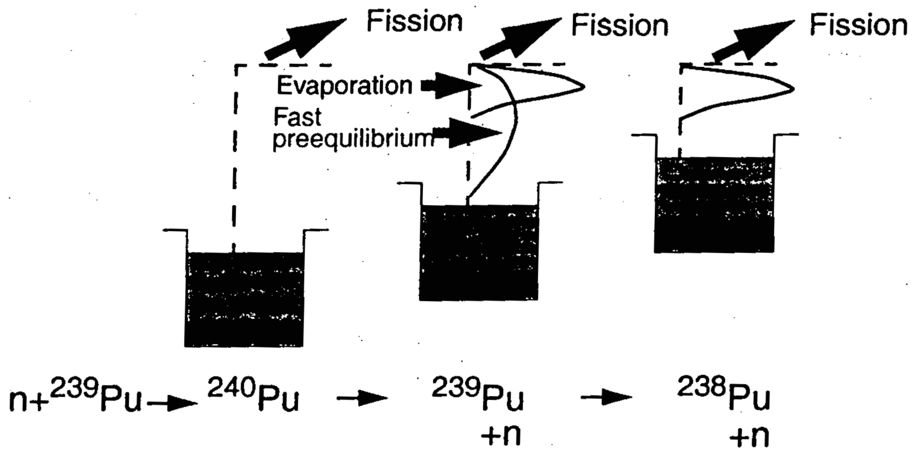
- Coupled-channel optical potential for neutrons
- Experimental fission data constrain calculations:

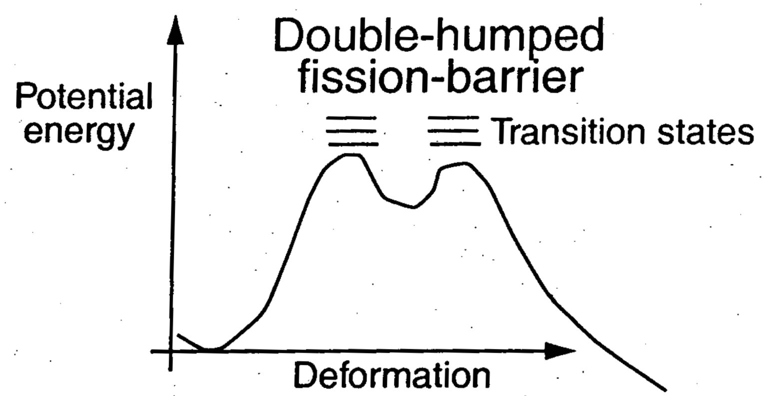
— ^{240,239}Pu barriers from (n,f)

— ^{238}Pu barrier from (^{3}He,df)

— Moller-Nix calculated barriers

- Angular momentum effects important; γ-ray branching ratios from measurements (discrete levels) and from Giant Resonance models

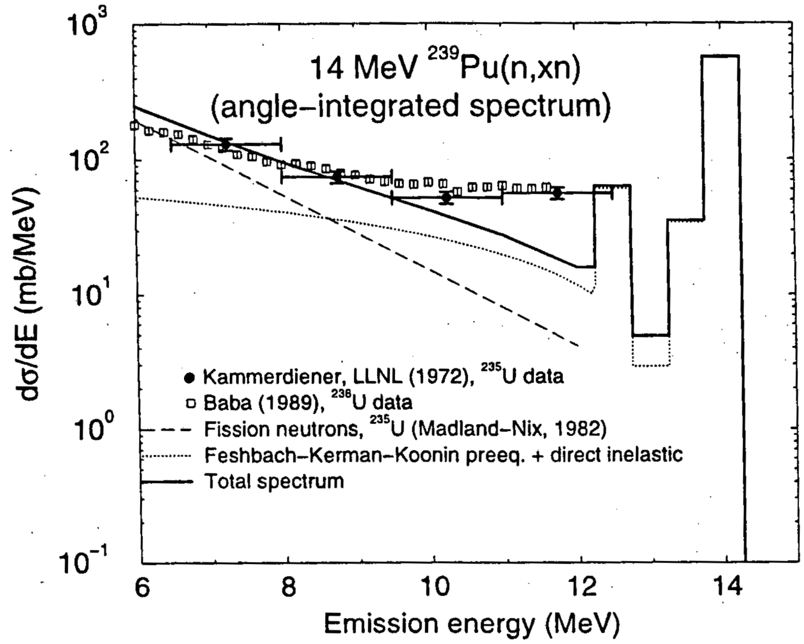




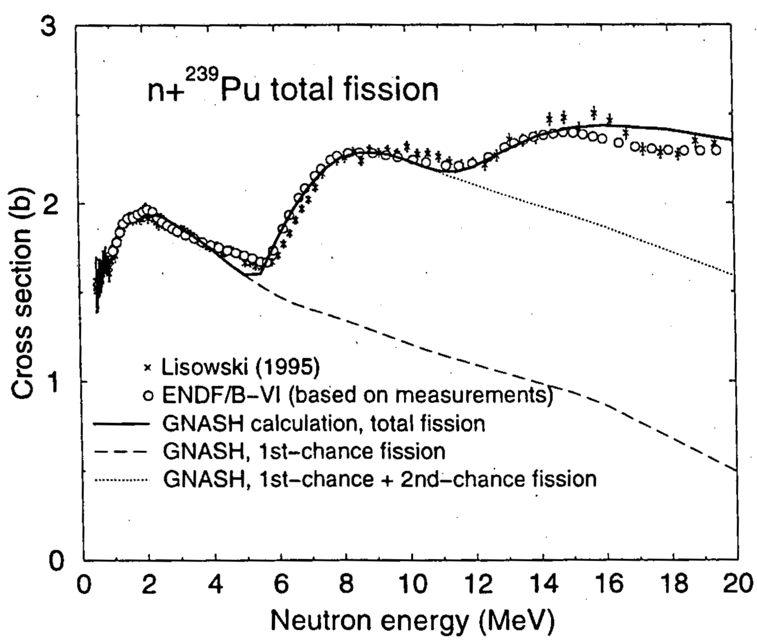
Los Alamos

Testing nuclear model calculations using measured data

Inelastic scattering, in competition with (n,2n), can be validated through comaprisons with high-energy neutron emission data:



Fission, in competition with (n,2n), is important to model correctly. Fission barriers initially taken from measurements, but subsequently tuned to fit (n, xf) data:

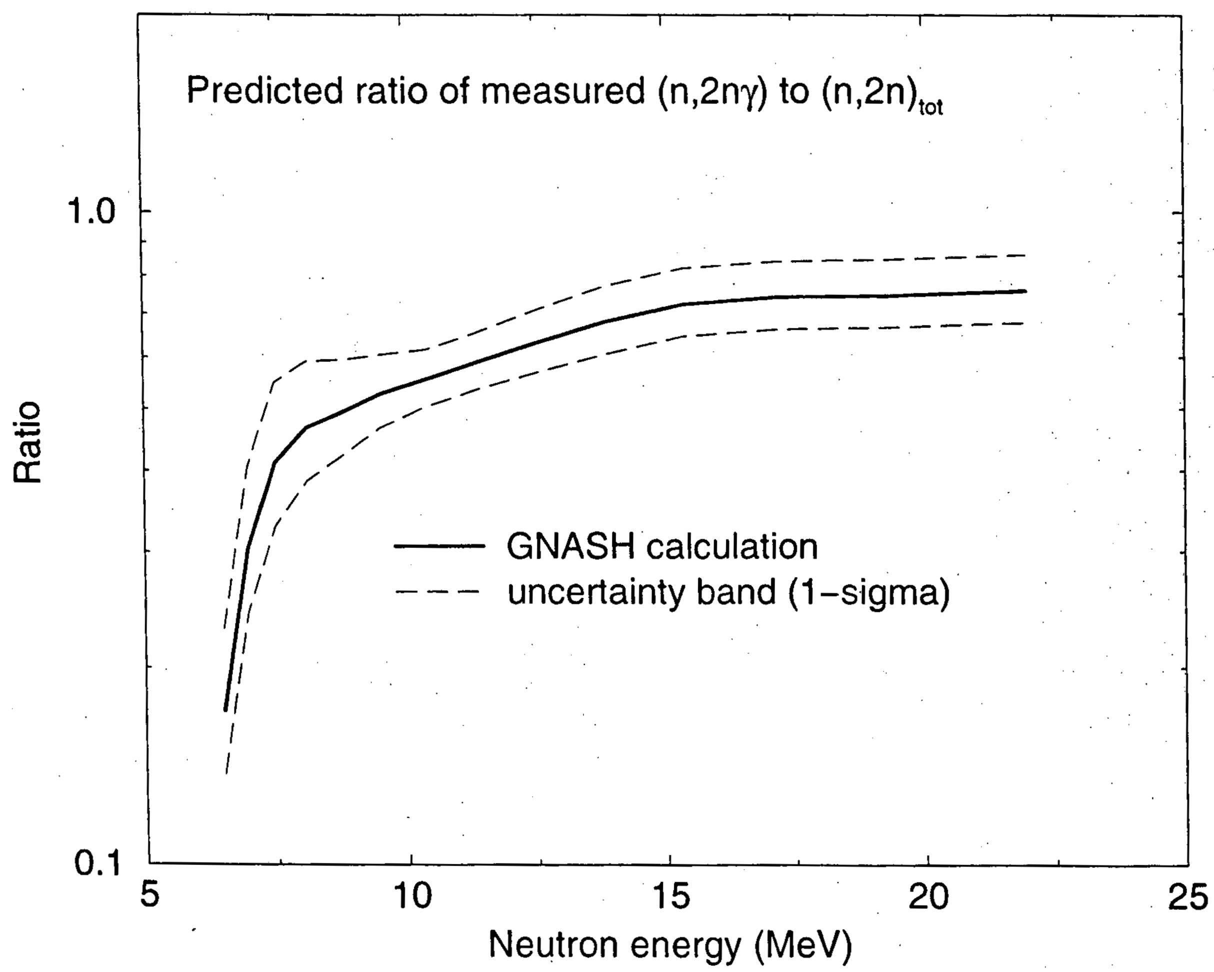


Theory contribution to $(n, 2n)$

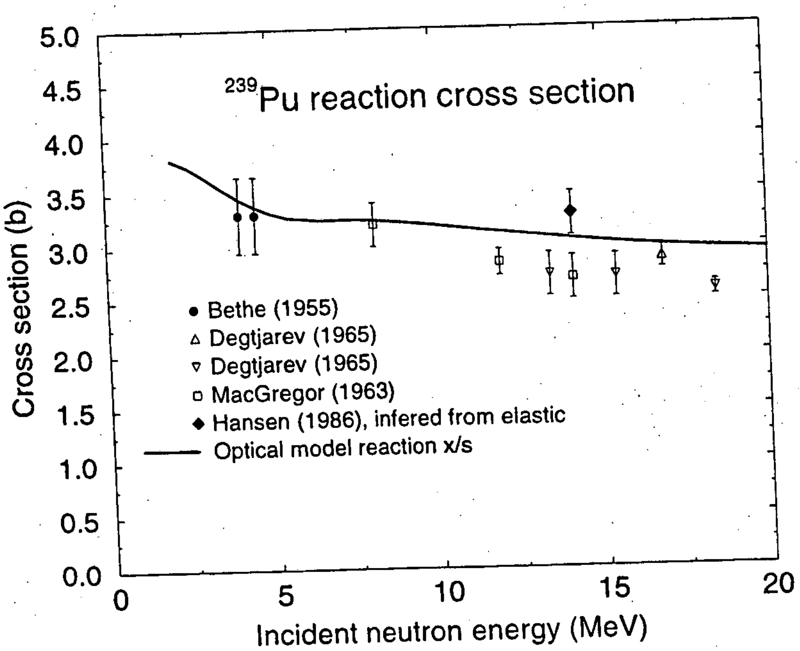
The GEANIE experiment measured 6 independent γ-rays. To infer the total $(n, 2n)$ cross section, we use :

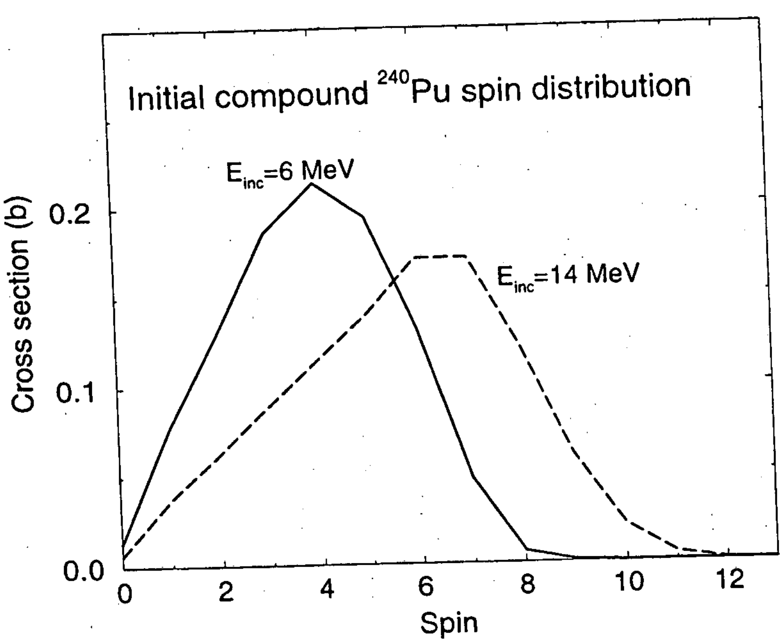
$$\sigma(n, 2n) = \sum_i \sigma_i^{\text{expt}}(n, 2n\gamma) \left[\frac{\sigma^{\text{theory}}(n, 2n)}{\sum_i \sigma_i^{\text{theory}}(n, 2n\gamma)} \right]$$

By summing 6 γ-rays, we use as much of the experimental information as possible, and mitigate against weaknesses in the predictions of individual gamma-rays



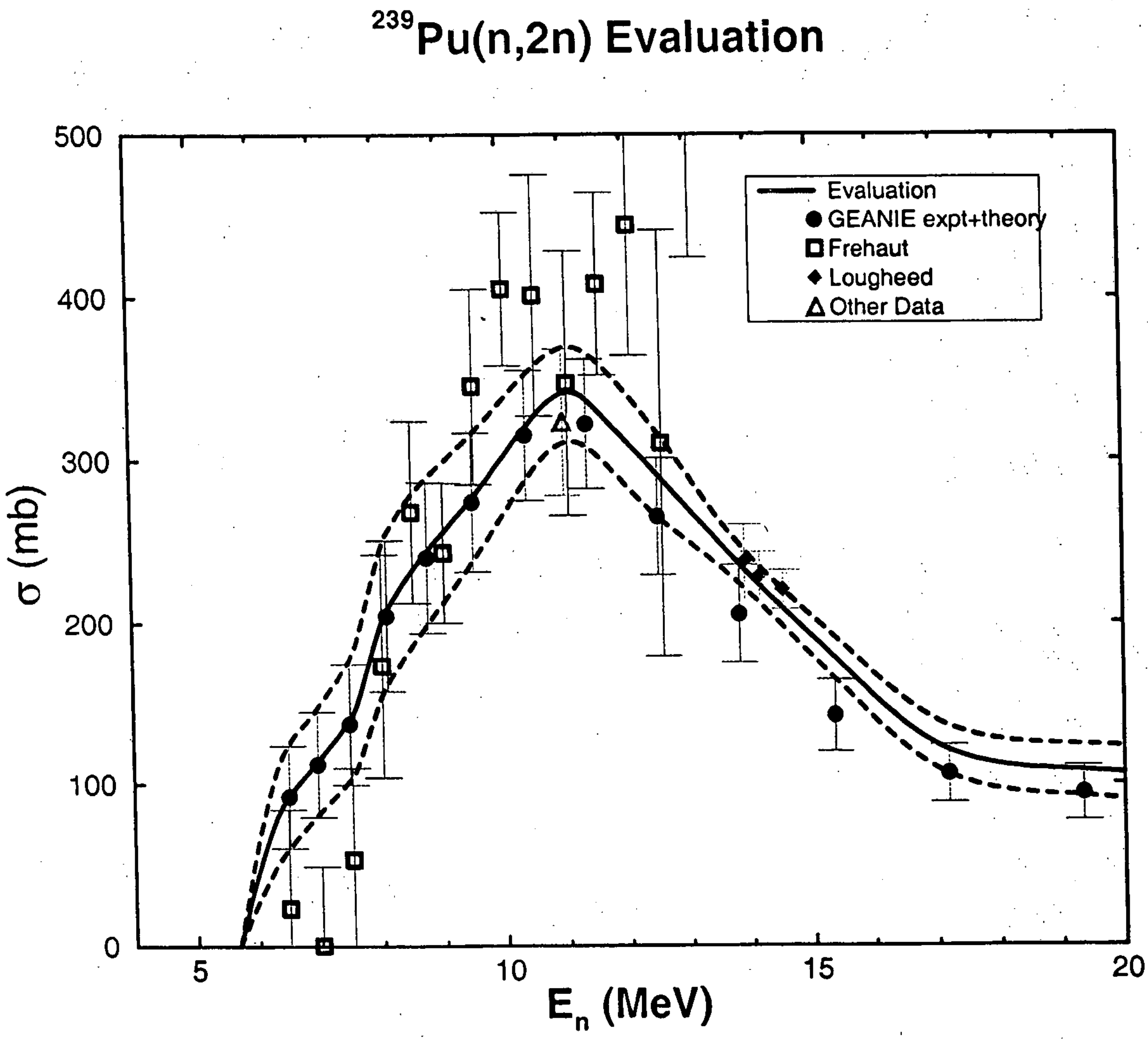
Optical model for n+^{239}Pu





Evaluated $^{239}Pu(n,2n)$ *data*

- Use GEANIE data, and Lougheed data near 14 MeV
- Do not use Frehaut data because of threshold behaviour
- At 11 MeV, use LLNL Anderson/Bauer/Navratil value
- Perform a covariance analysis of these data

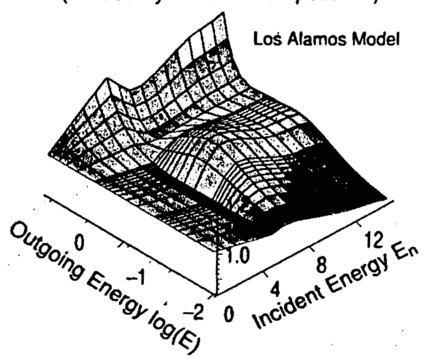


New n + ^{239}Pu ENDF cross section evaluation, T-16

(experiment and theory both crucial)

Prompt fission neutrons

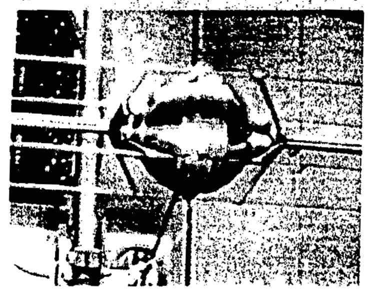
(divided by the thermal spectrum)

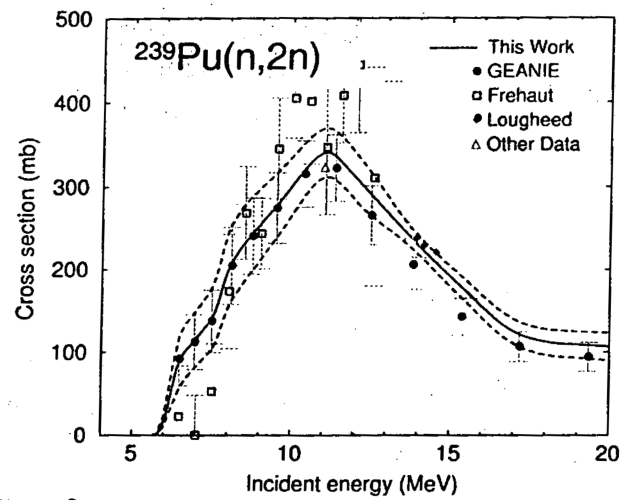


Jezebel critical assembly

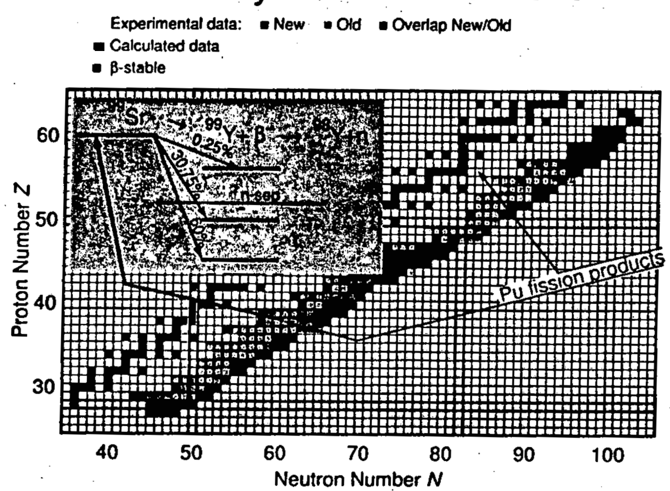
k_{eff} = 0.998 = calc/exp

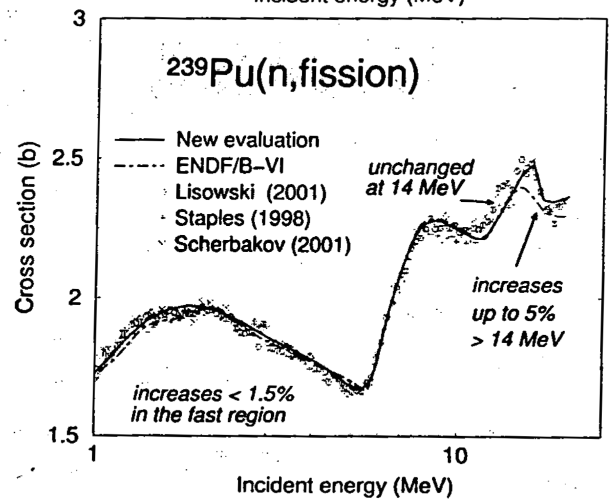
(previous value = 0.996)



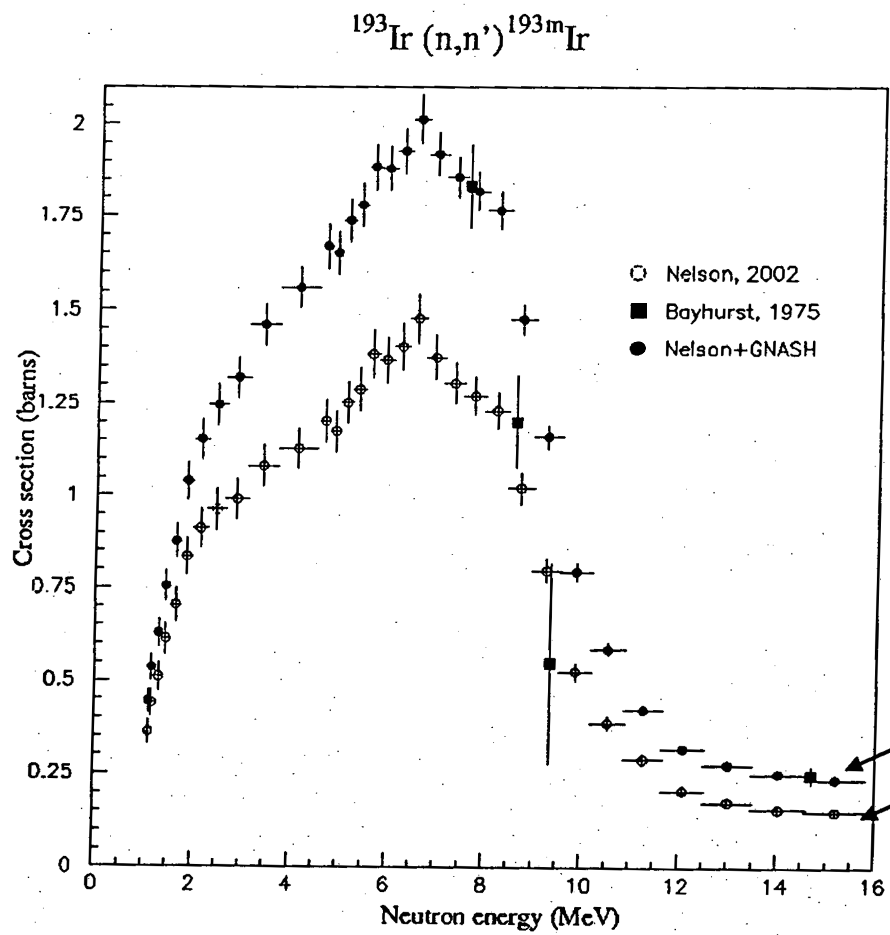


Delayed fission neutrons



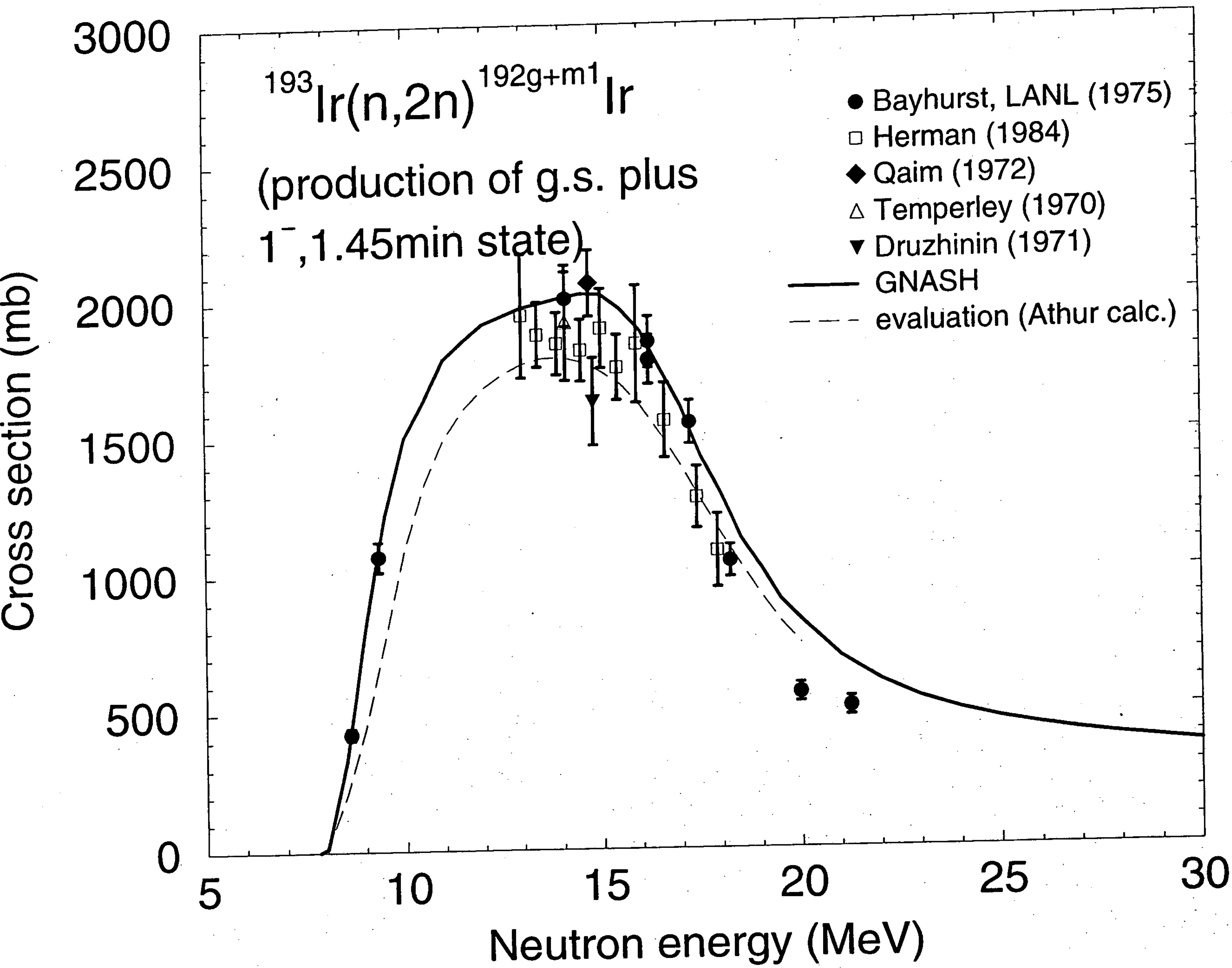


$^{193}Ir(n,n')$, 5.5-, 10 day isomer production

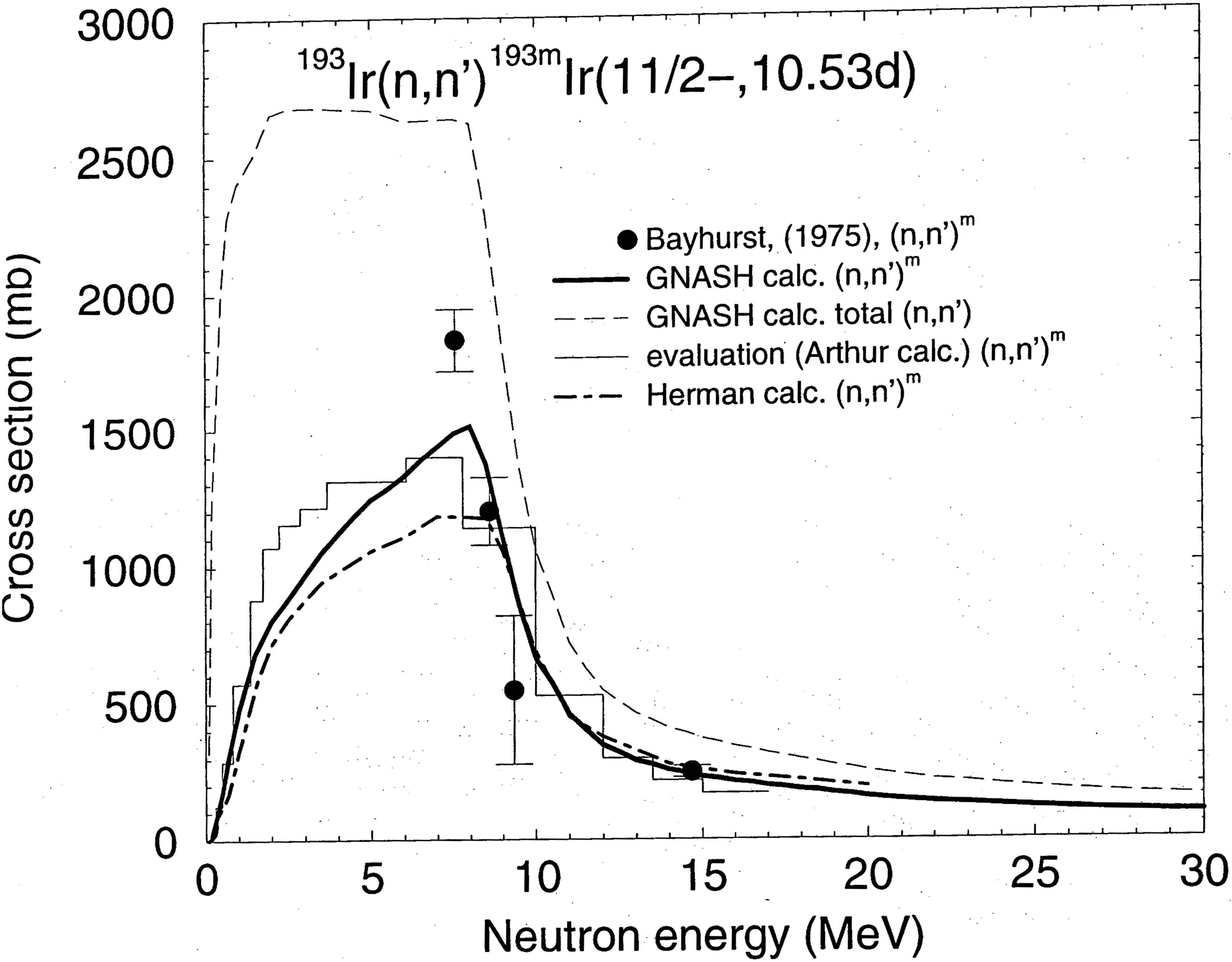


GEANIE measurement augmented by theory predictions of unmeasured gamma-rays

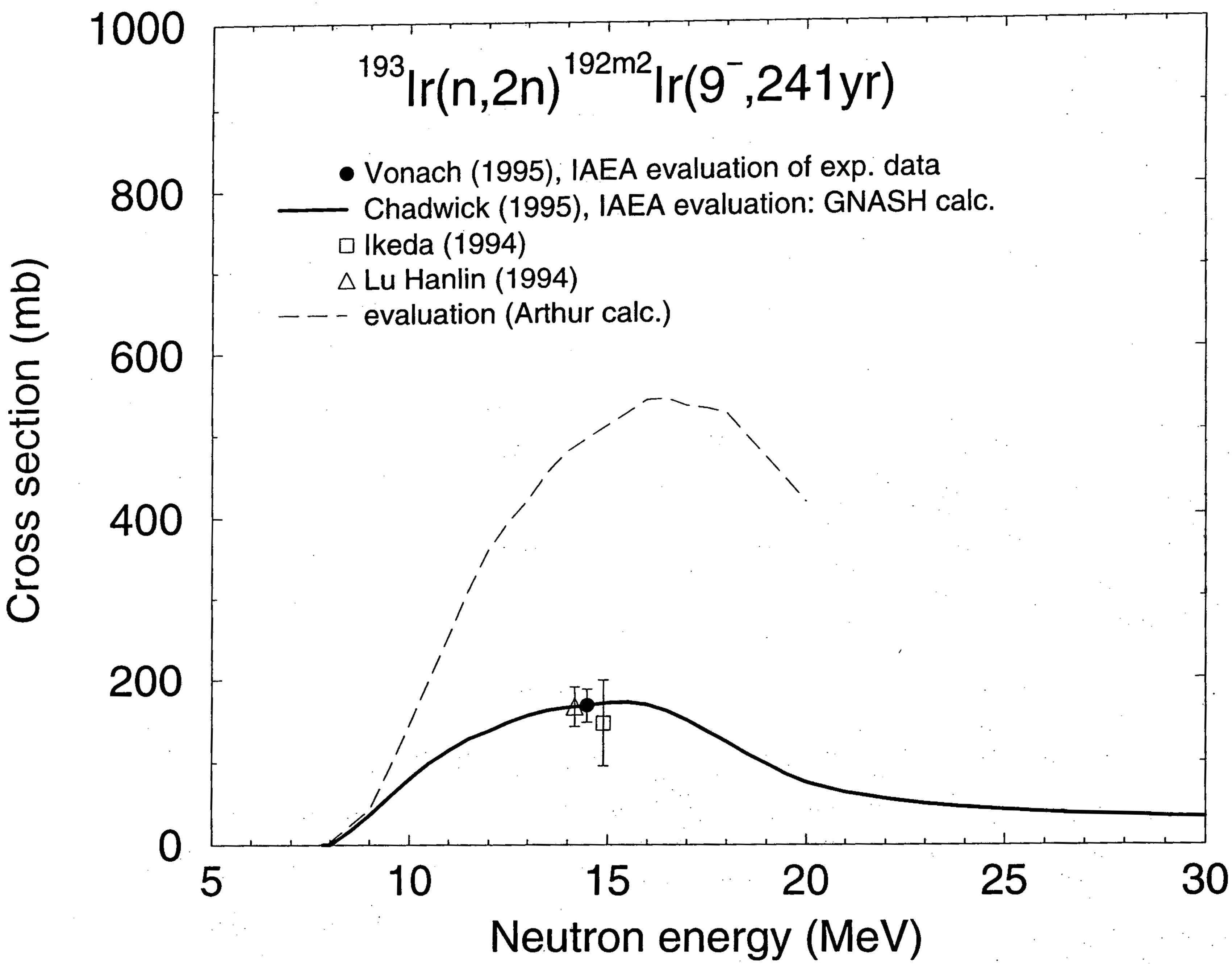
GEANIE-measurement



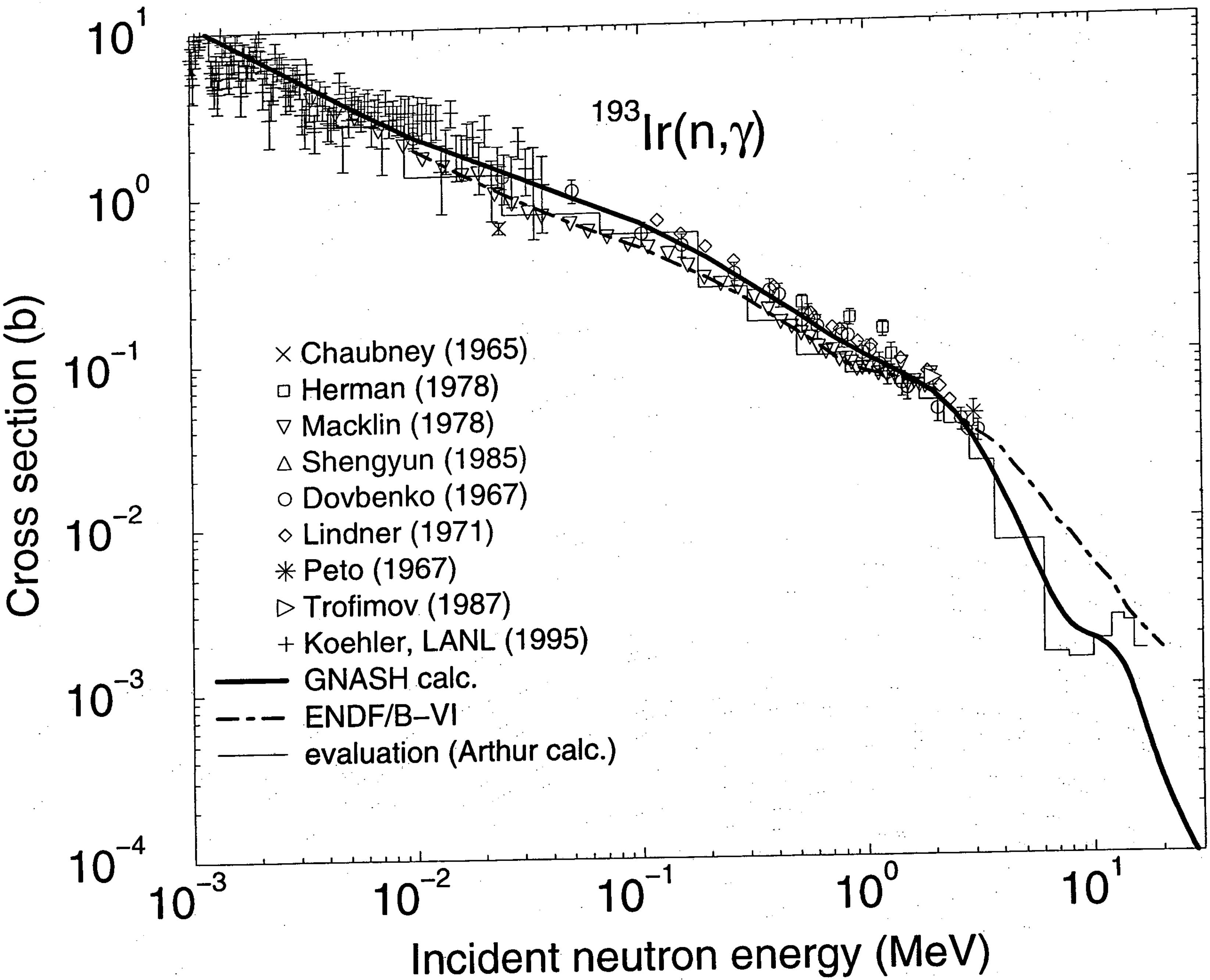
$^{193}Ir(n,2n)^{192g+m1}Ir$
(production of g.s. plus
1^-,1.45min state)
Bayhurst, LANL (1975)
Herman (1984)
Qaim (1972)
Temperley (1970)
Druzhinin (1971)
GNASH
evaluation (Athur calc.)
Cross section (mb)
Neutron energy (MeV)
0
500
1000
1500
2000
2500
3000
5
10
15
20
25
30



$^{193}Ir(n,n')^{193m}Ir(11/2-,10.53d)$
Bayhurst, (1975), (n,n')^m
GNASH calc. (n,n')^m
GNASH calc. total (n,n')
evaluation (Arthur calc.) (n,n')^m
Herman calc. (n,n')^m
Cross section (mb)
Neutron energy (MeV)
3000
2500
2000
1500
1000
500
0
0
5
10
15
20
25
30



$^{193}Ir(n,2n)^{192m2}Ir(9^-,241yr)$
Vonach (1995), IAEA evaluation of exp. data
Chadwick (1995), IAEA evaluation: GNASH calc.
Ikeda (1994)
Lu Hanlin (1994)
evaluation (Arthur calc.)
Cross section (mb)
Neutron energy (MeV)
1000
800
600
400
200
0
5
10
15
20
25
30



$^{193}Ir(n,\gamma)$
Cross section (b)
Incident neutron energy (MeV)
10^{1}
10^{0}
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-3}
10^{-2}
10^{-1}
10^{0}
10^{1}
× Chaubney (1965)
□ Herman (1978)
▽ Macklin (1978)
△ Shengyun (1985)
○ Dovbenko (1967)
◇ Lindner (1971)
✳ Peto (1967)
▷ Trofimov (1987)
+ Koehler, LANL (1995)
GNASH calc.
ENDF/B–VI
evaluation (Arthur calc.)

Hybrid Monte Carlo Simulation (HMS) Preequibrium Model

- Blann (PRC54, 1341, 1996): *dxs* energy spectra
- Blann and Chadwick (PRC57, 233, 1998): *ddxs* energy-angle spectra
- Blann and Chadwick (PRC6203,4604 (200)): cluster projectiles
- Chadwick and Blann (ND2001): ang mom, recoils,cm->lab

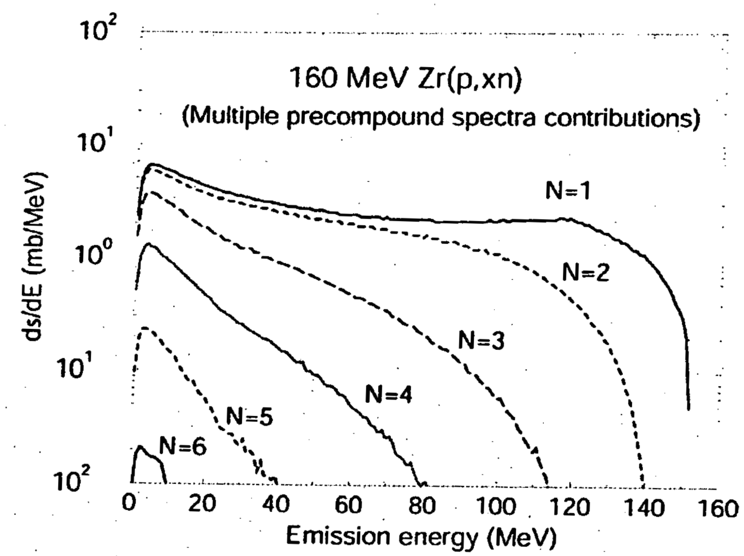
- Included in Monte Carlo version of ALICE (Blann)

- Implemented in ddxs.f (Chadwick), and distributed via WPEC nuclear models collaboration (Herman, Oblozinsky,...)

- Recently used in a Los Alamos project to create an activation cross section database, including isomer production

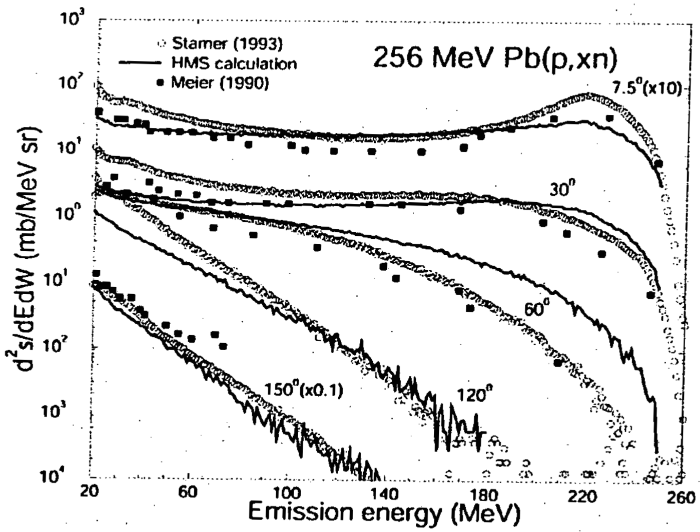
Hybrid Monte Carlo Simulation (HMS): Physics advantages

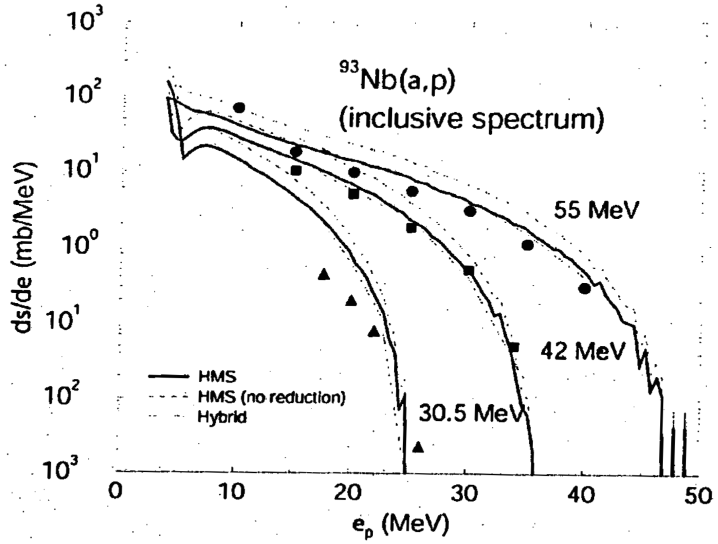
- Event-based, easily allowing exclusive cross sections to be determined and gates to be set *(correlations)*
- Each successive nucleon scattering produces a new 3-exciton configuration (avoiding higher order p-h densities inconsistent with 2-body scattering (Bisplinghoff))
- Multiple preeq. for unlimited particle emission
- Comprehensive modeling of all reaction mechanisms
- Recoils, and cm->lab transformations



Hybrid Monte Carlo Simulation (HMS): Examples of emission spectra modeling

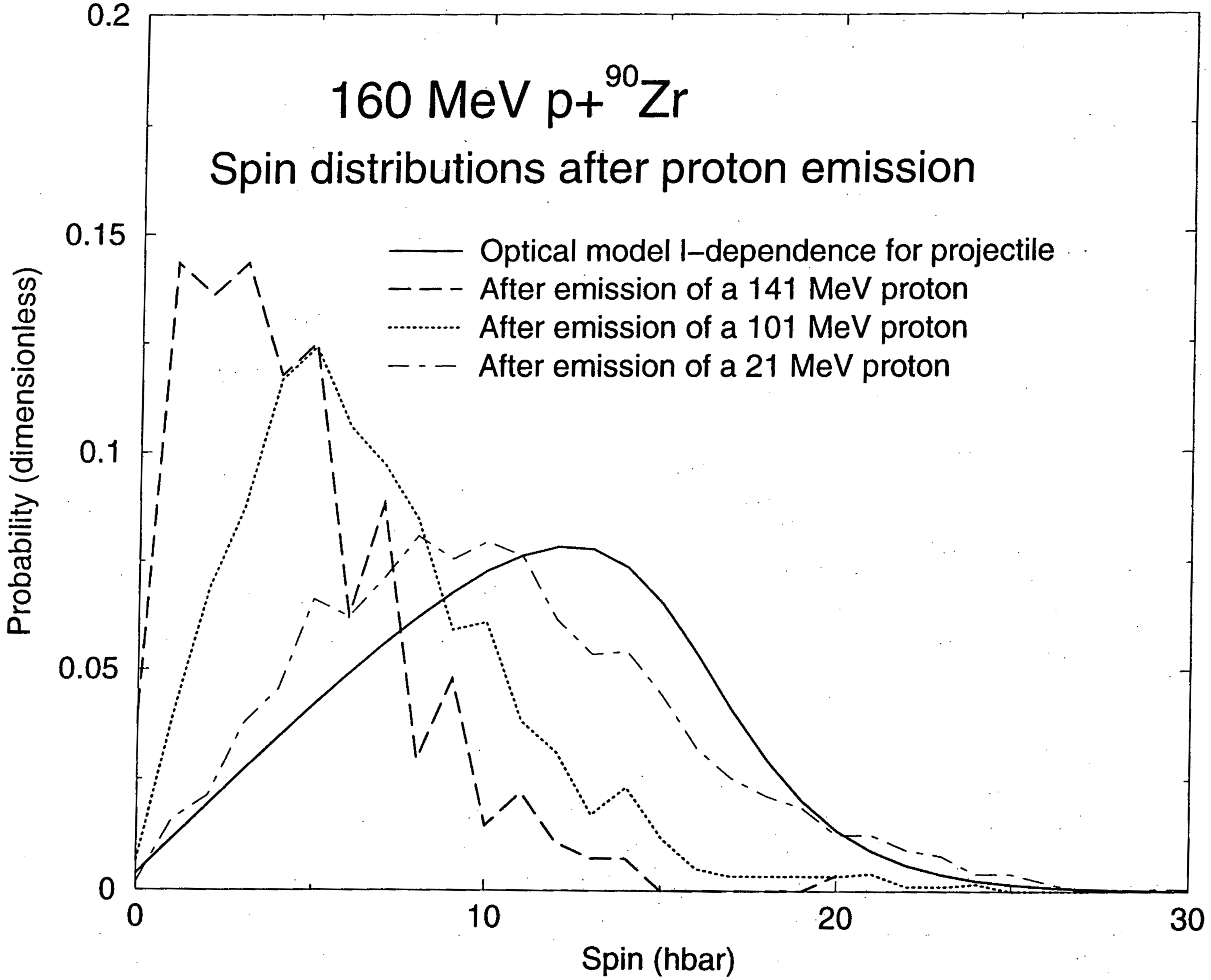
- Nucleon spectra: Theory accounts for the energy-and angular-dependence of the spectra
- Cluster projectiles: 60-70% of the reaction cross sections lead to the collisions in which the alpha might ``dissolve" in the field of the nucleus



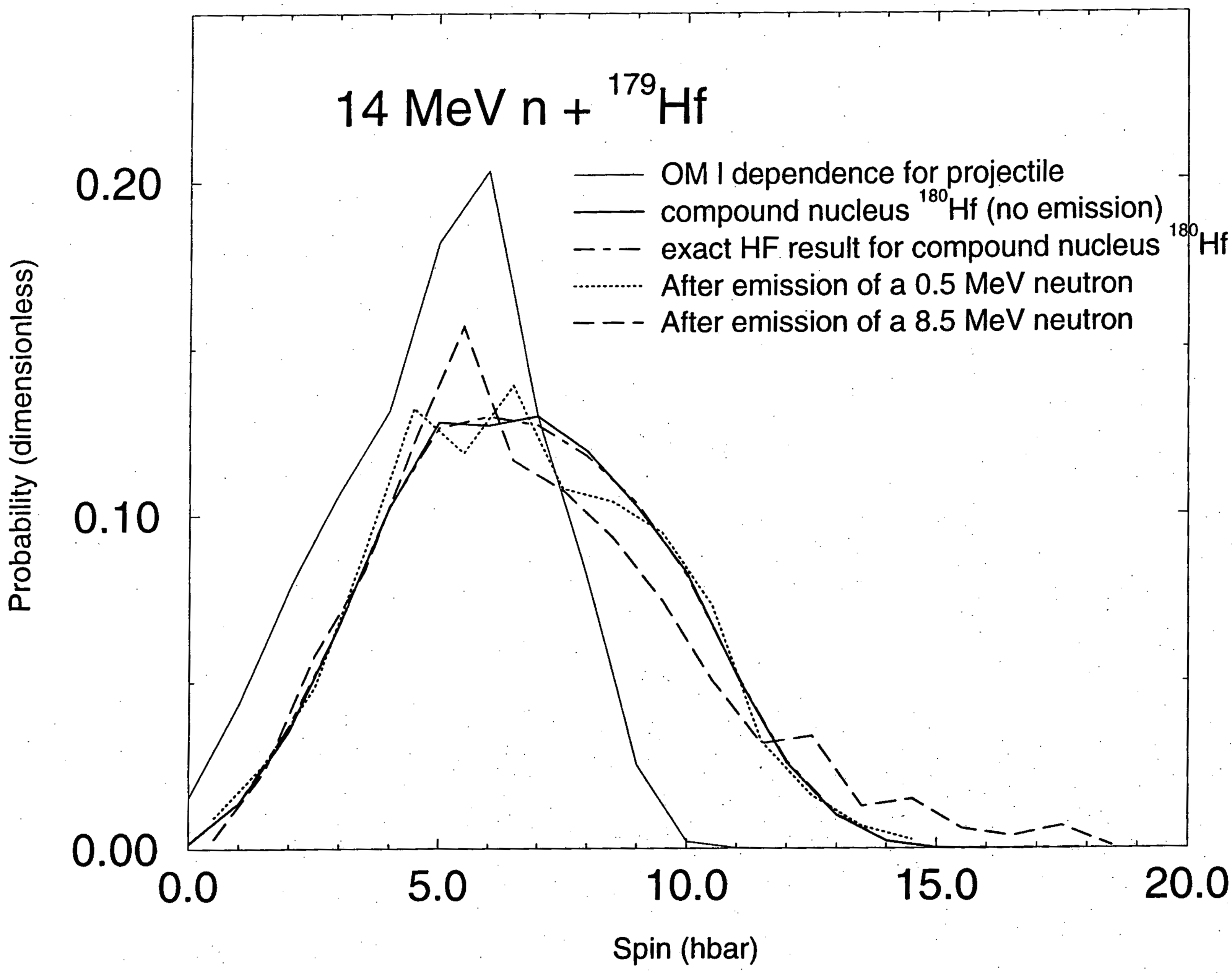


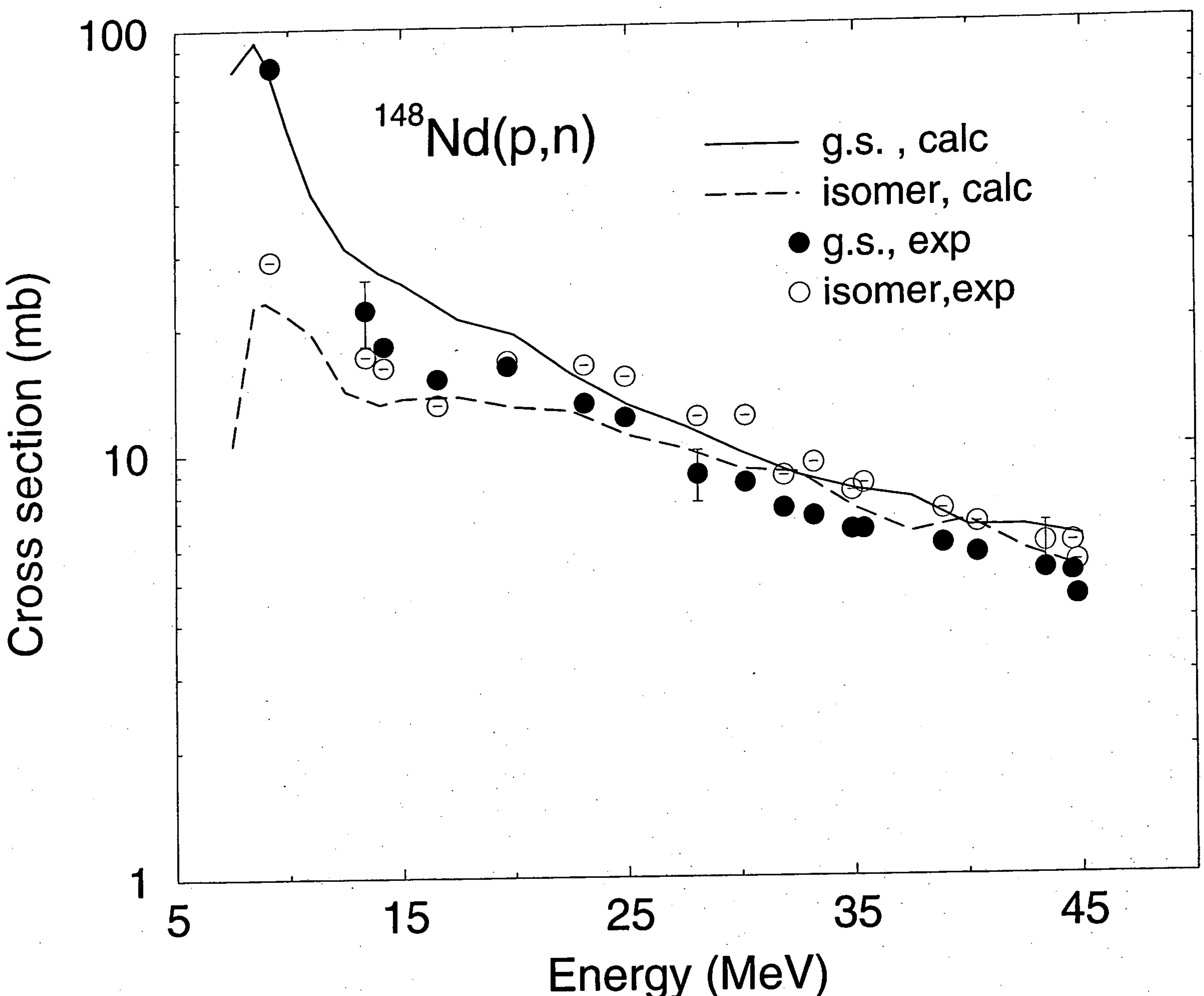
Hybrid Monte Carlo Simulation (HMS): Angular momentum spin transfer (with Oblozinsky)

- Needed to couple HMS to Hauser-Feshbach codes (*e.g. GNASH, EMPIRE*)
- Important for modeling spin-dependent observables
  - isomer production
  - discrete gamma-rays in final decaying nuclei (and nuclear reaction mechanisms with GEANIE)
  - fission probabilities
- We assume semi-classical **r x p**, with the impact parameter taken from a Fermi distribution, or inferred from the OM
- As the emission energy increases, corresponding to typically forward-peaked angular distribution preequilibrium particles, the spin distribution of the residual nucleus peaked at increasingly low spins

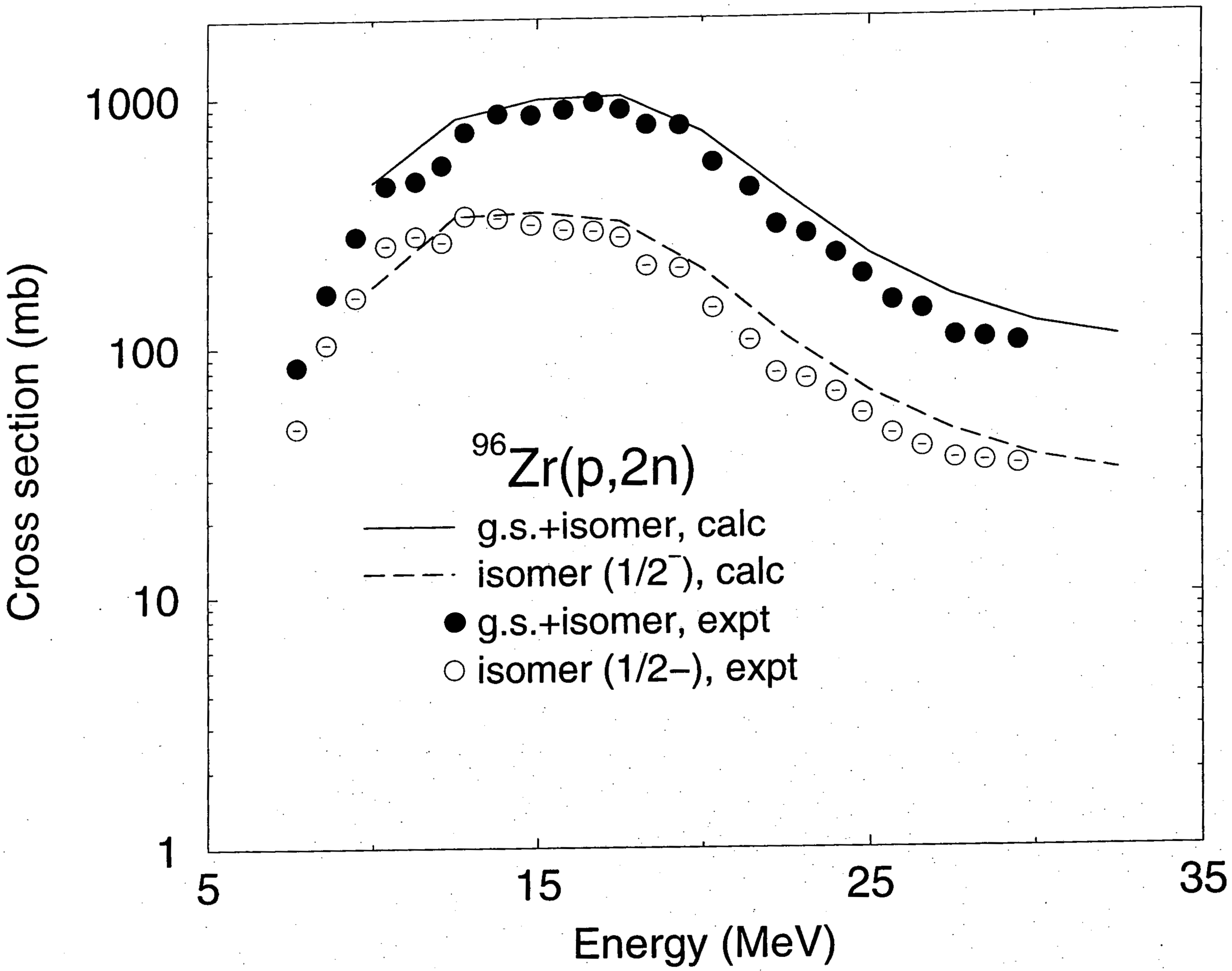


160 MeV p+^{90}Zr
Spin distributions after proton emission
Optical model l–dependence for projectile
After emission of a 141 MeV proton
After emission of a 101 MeV proton
After emission of a 21 MeV proton
Probability (dimensionless)
Spin (hbar)
0.2
0.15
0.1
0.05
0
0
10
20
30


14 MeV n + ^{179}Hf
OM l dependence for projectile
compound nucleus ^{180}Hf (no emission)
exact HF result for compound nucleus ^{180}Hf
After emission of a 0.5 MeV neutron
After emission of a 8.5 MeV neutron
Probability (dimensionless)
0.20
0.10
0.00
0.0
5.0
10.0
15.0
20.0
Spin (hbar)



148Nd(p,n)
g.s. , calc
isomer, calc
g.s., exp
isomer,exp
Cross section (mb)
Energy (MeV)
100
10
1
5
15
25
35
45



^{96}Zr(p,2n)
g.s.+isomer, calc
isomer (1/2$^-$), calc
g.s.+isomer, expt
isomer (1/2–), expt
Cross section (mb)
Energy (MeV)
1000
100
10
1
5
15
25
35